
1-Naphthol

CAS # 90-15-3

Test plan justification**Bayer CropScience LP**July, 2003

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2003 JUL 28 PM 1:02**Executive Summary**

Bayer CropScience LP (Bayer) hereby submits for review and public comment their test plan for 1-naphthol under the Environmental Protection Agency's High Production Volume (HPV) Chemical Challenge Program.

1-naphthol, is used as: a pigment, as well as an additive, to help "shade" products; a dye which is used in inks and coatings; a hair dye without further processing, as well as used in production of hair dyes; an additive for polymers to keep the kettle clean allowing for many more batches to be produced before they have to shut down and wash out; and several specialty applications.

In consideration of animal welfare concerns to minimize the use of animals in the testing of chemicals, Bayer has conducted a thorough literature search for all available data, published and unpublished. It has also performed an analysis of the adequacy of the existing data. Existing data indicates that this chemical is of moderate concern for aquatic toxicity, low concern as Persistent Organic Pollutants (POP), moderate concern for skin and eye irritation, and low concern for mammalian toxicity, carcinogenicity and allergic skin reactions. Bayer concludes that there is sufficient data on 1-naphthol and no additional testing is recommended for purposes of the HPV Program.

Data Review

Physicochemical properties:

The properties of 1-naphthol can be found in Handbooks such as CRC Handbook of Chemistry and Physics and The Merck Index. 1-naphthol; is a solid at ambient temperatures, with a melting point of 95°C and boiling point of 288°C. The measured octanol/water partition coefficient is 3 and it has limited solubility in water. Data is available for all endpoints, no additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

Environmental Fate:

Photodegradation was calculated to have half-life of 1.9 hours. Fugacity modeling demonstrates partitioning to the soil and water compartments. A Guideline Biodegradation study demonstrates ready biodegradability. A water stability study demonstrated that dissolved oxygen promotes aqueous-phase oxidative transformation of 1-naphthol which is controlled by pH and ionic strength. The fraction of 1-naphthol transformed is negligible below pH 6.5; increasing pH > 7.0 and leveling off around pH 9.0. In the absence of dissolved oxygen, 1-naphthol is stable at all solution conditions (pH and ionic strength). No additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

Ecotoxicology:

Aquatic studies have been performed on several species of fish, on aquatic invertebrates and algae. Fish appear to be the most sensitive species: LC₅₀ = 0.75 mg/l (*L. macrochirus*) to 4.24 mg/l (*P. promelas*). There are also chronic studies on *Daphnia magna* and algae. No additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

Mammalian Toxicology:

Toxicity studies show that 1-naphthol is of low acute toxicity by all routes of exposure (oral LD₅₀ = 1000-3300 mg/kg; inhalation LC₅₀ > 97 mg/m³; and dermal LD₅₀ > 10,000 mg/kg) (See Table 1 and IUCLID document).

There are multiple studies to fill the Mutagenicity endpoints, both *in vitro* and *in vivo*. All results were negative (See Table 1 and IUCLID document).

There are several repeated dose toxicity studies (sub-acute, sub-chronic and chronic) by oral and dermal route of exposure which demonstrate a low concern for toxicity (See Table 1 and attached IUCLID document).

A two generation Fertility study was performed as well as several Developmental studies, also demonstrating a low concern for toxicity (See Table 1 and attached IUCLID document).

There is data to cover all SIDS endpoints, no additional testing is proposed for purposes of the HPV Program (See Table 1 and IUCLID document).

“Beyond SIDS” Endpoints:

Studies have been performed to investigate skin and eye irritation skin sensitization potential. A carcinogenicity study was also performed demonstrating no significant increases in tumors in either sex compared to control groups (See Table 2 and IUCLID document).

Conclusion

Existing data indicates that this chemical is of moderate concern for aquatic toxicity, low concern as Persistent Organic Pollutants (POP), moderate concern for skin irritation, low concern for allergic skin reaction, and low concern for mammalian toxicity and carcinogenicity. Bayer concludes that there is sufficient, reliable data on 1-naphthol and no additional testing is recommended for purposes of the HPV Program.

Table 1. Available data for 1-naphthol (CAS# 90-15-3)

Endpoint	Result	Method*
Physical-Chemical Data		
Melting Point	95 °C	Handbook data
Boiling Point	288 °C @ 1000 hPa	Handbook data
Vapour Pressure	36 hPa @ 25 °C	Handbook data
Partition Coefficient (logP _{ow})	3 @ 23 °C	OECD 117
Water Solubility	Insoluble	Handbook data
Environmental Fate		
Photodegradation	T ½ = 1.9 hours	SRC calculation
Fugacity	Air = 0.07 % Water = 39.8 % Soil = 59.8% Sediment = 0.3%	Fugacity Level III modeling
Biodegradability	96% after 14 D	MITI test
Water Stability	Stable @ pH ≤ 6.5; Increased transformation with increased pH	Karthikenyan, 2000
Ecotoxicology		
Acute Fish Toxicity (96 hrs)	<i>L. macrochirus</i> LC ₅₀ = 0.75 mg/l <i>P. promelas</i> LC ₅₀ = 4.24 mg/l	EPA OPP 72-1 EPA OTS 797.1400
Acute Invertebrate Toxicity (48 hrs)	<i>Daphnia magna</i> EC ₅₀ = 3.53 mg/l	OECD 202
Algal Toxicity (20 days)	<i>Chlorella vulgaris</i> EC ₅₀ = 20-50 mg/l	Megharaj, 1990
Mammalian Toxicology		
Acute Toxicity	1000-3300 mg/kg bw > 97 mg/m ³ > 10,000 mg/kg	Oral, rat Inhalation, rat Dermal, rabbit
Mutagenicity	Negative	Ames test
Chromosome Aberration	Negative	Micronucleus assay (rat, gavage and mouse, i.p.)
Repeated Dose Toxicity	NOAEL = 130 mg/kg/d	OECD 408 (13 week, oral, rat)
Reproductive Toxicity	NOAEL = 0.5%	Two generation study, dermal, rat
Developmental Toxicity	NOAEL (developmental) = 400 mg/kg/d NOAEL (maternal) = 20 mg/kg/d	OECD 414 Rat, gavage

* Robust summaries and References can be found in the IUCLID document.

Table 2. "Beyond SIDS" data for 1-naphthol (CAS# 90-15-3)

Endpoint	Result	Method*
Skin Irritation	Irritating	Draize Test (rabbit)
Eye Irritation	Irritating	Draize Test (rabbit)
Dermal Sensitization	Not sensitizing	Guinea Pig Maximization Test
Carcinogenicity	Negative	2 year, dermal (rat and mouse)

* Robust summaries and References can be found in the IUCLID document.

Table 3. Test Plan for 1-naphthol (CAS# 90-15-3)

Endpoint	Data Availability	Acceptable	Planned testing
Physical-Chemical Data			
Melting Point	✓	✓	
Boiling Point	✓	✓	
Vapour Pressure	✓	✓	
Partition Coefficient (logP _{ow})	✓	✓	
Water Solubility	✓	✓	
Environmental Fate			
Photodegradation	✓	✓	
Fugacity	✓	✓	
Biodegradability	✓	✓	
Water Stability			
Ecotoxicology			
Acute Fish Toxicity	✓	✓	
Acute Invertebrate Toxicity	✓	✓	
Algal Toxicity	✓	✓	
Mammalian Toxicology			
Acute Toxicity	✓	✓	
Mutagenicity	✓	✓	
Chromosome Aberration	✓	✓	
Repeated Dose Toxicity	✓	✓	
Reproductive Toxicity	✓	✓	
Developmental Toxicity	✓	✓	

✓ = data available and considered adequate.

References

- Karthikenyan KG. & Chorover J. 2000. Environ. Sci. Technol. 34:2939-2946.
- Megharaj M. et al. 1990. Interaction effects of carbaryl and its hydrolysis product, 1-naphthol, towards three isolates of microalgae from rice soil. Agricul.Ecosystems and Environ. 31:293-300.
- Poole A. and Buckley P. 1989. 1-Naphthol - single and repeated dose (30-day) oral toxicity studies in the mouse. Fd. Chem. Toxic. 27(4):233-238.

Additional References can be found in the IUCLID document.